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# WIENER INDEX OF SOME PATH RELATED GRAPHS

**A. SUMATHI**

Department of Mathematics, Seethalakshmi Ramaswami College, Tiruchirappalli, Tamil Nadu, India

## ABSTRACT

The Wiener index is one of the oldest molecular-graph-based structure-descriptors. It was first proposed by American Chemist Harold Wiener in 1947 as an aid to determine the boiling point of paraffin. The study of Wiener index is one of the current areas of research in mathematical chemistry. It also gives good correlations between Wiener index (of molecular graphs) and the physico chemical properties of the underlying organic compounds. That is, the Wiener index of a molecular graph provides a rough measure of the compactness of the underlying molecule. The Wiener index W(G) of a connected graph G is the sum of the distances between all pairs (ordered) of vertices of G. $W(G) = \frac{1}{2}\sum_{u,v} d(u,v)$. In this paper, the researcher finds the Wiener index of some path related graphs like $m^{th}$ power of path graph, $m_i^{th}$ power of path graph $\sigma$ mountain, $\sigma$ hill.

**KEYWORDS:** Adjacency Matrix, MATLAB, Wiener Index

## 1. INTRODUCTION

The Wiener index **W (G)** is a distance-based topological invariant much used in the study of the structure-property and the structure-activity relationships of various classes of biochemically interesting compounds introduced by Harold Wiener in 1947 for predicting boiling points b. p of alkanes based on the formula

$$b.p = \alpha W + \beta w(3) + \gamma$$

Where $\alpha, \beta, \gamma$ are empirical constants, and w(3) is called path number. It is defined as the half sum of the distances between all pairs of vertices of G.

$$W(G) = \frac{1}{2}\sum_{u,v\in G} d(u,v)$$

Where d (u, v) is the number of edges in a shortest path connecting the vertices u & v in G[5]

**Notation**

$$W(G) = \frac{1}{2}\sum_{u,v\in G} d(u,v) = \sum_{u<v} d(u,v) = \sum_{i<j} d(u_i,u_j)$$

## 2. DEFINITIONS AND PRELIMINARIES

Our notation is standard and mainly taken from standard books of graph theory [1]. In this paper, the researcher considers finite, nontrivial, simple and undirected graphs. For a graph G, the researcher denotes by V(G) and E(G), its

vertex and edge sets, respectively.

**Definition 2.1:** $m^{th}$ power of the path $P_n$ [2]

Let $P_n$ denote a path of length n-1. The $m^{th}$ power of the path $P_n$ is obtained from $P_n$ by adding edges that join all vertices u and v whose distance is m. It is denoted by $P_n^m$

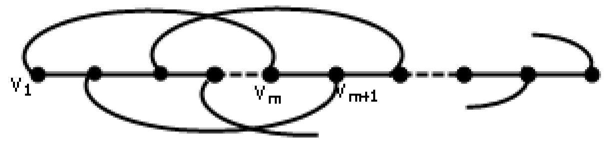



**Figure 1**

**Definition 2.2:** $m_i^{th}$ power of the path $P_n$

Let $P_n$ denote a path of length n-1. The $m_i^{th}$ power of the path $P_n$ is obtained from $P_n$ by adding edges from every vertex u to the vertices of distance is i, where m-1≤ i ≤ m+1. It is denoted by $P_n^{m_i}$

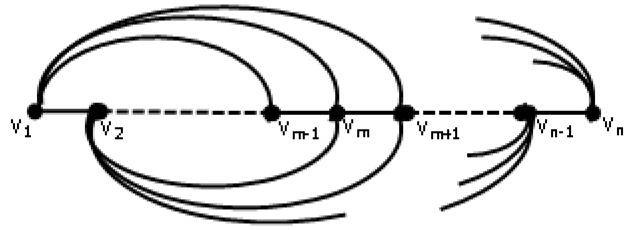


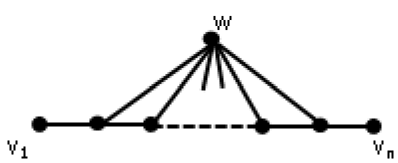

**Figure 2**

**Definition 2.3:** σ mountain [3]

Let $P_n$ denote a path of length n-1. The graph σ mountain is obtained from the path $P_n$, $n \geq 3$,the vertex set $\{v_1,v_2,\ldots.v_n,w\}$ and the edge set is $v_i\ v_{i+1}$ for $1 \leq i \leq n-1$ and $wv_i$ for $2 \leq i \leq n-1$ and any other pair of vertices is not joined by an edge.

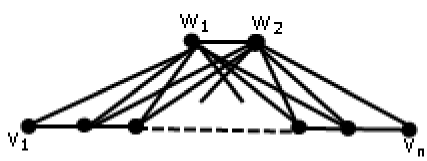
**Definition 2.4:** σ hill [3]

Let $P_n$ denote a path of length n-1. The graph σ hill is obtained from the path $P_n$, $n \geq 2$, the vertex set $\{v_1,v_2,\ldots.v_n,w_1,w_2\}$ and the edge set is $v_i\ v_{i+1}$ for $1 \leq i \leq n-1$, $w_1w_2$, $w_1v_i$, for $1 \leq i \leq n-1$ , $w_2v_i$ for $2 \leq i \leq n$ any other pair of vertices is not joined by an edge.




σ mountain

**Figure 3**




σ hill

**Figure 4**

The Program for finding Wiener index of any graphs given in [4]. The following program computes the Adjacency matrix of above graphs through MATLAB.

## 3. PROGRAM FOR FINDING WIENER INDEX OF GRAPHS

**Program 3.1:**

%This MATLAB Program calculates the Adjacency matrix of $m^{th}$ power of the path $P_n$

%Adjacency matrix of $m^{th}$ power of the path $P_n$

```
n= input('Path with vertices n=');
m= input('Jump with a distance m=');
A=[];
for i=1:n-1
    A(i,i+1)=1;A(i+1,i)=1;
      if i+m<=n
    A(i,i+m)=1;A(i+m,i)=1;
    if i+m>n
    A(i,i+m)=0;A(i+m,i)=0;
    end
    end
end
A;
```

**Program 3.2:**

%This MATLAB Program calculates the Wiener index of $m_i^{th}$ power of the path $P_n$

%Adjacency matrix of $m_i^{th}$ power of the path $P_n$

```
n= input('Path with vertices n=');
m= input('No. of jumps m=');
A=[];
for i=1:n-1
    A(i,i+1)=1;A(i+1,i)=1;
    for j=1:m+1
    if i+j<=n
    A(i,i+j)=1;A(i+j,i)=1;
```

```
    if i+j>n
    A(i,i+j)=0;A(i+j,i)=0;
    end
    end
    end
end
A;
```

**Program 3.3:**

```
%This MATLAB Program calculates the Wiener index of σ mountain
%Program to find the Wiener index of σ mountain
%Adjacency matrix of σ mountain
n= input('Path with vertices n=');
A=[];
for i=1:n+1
for i=1:n-1
    A(i,i+1)=1;A(i+1,i)=1;
    for j=2:n-1
        A(j,n+1)=1;A(n+1,j)=1;
    end
end
end
A;
```

**Program 3.4:**

```
%This MATLAB Program calculates the Wiener index of σ hill
%Adjacency matrix of σ hill
n= input('Path with vertices n=');
A=[];
for i=1:n+2
   A(n+1,n+2)=1;A(n+2,n+1)=1;
```

```
for i=1:n-1
    A(i,n+1)=1;A(n+1,i)=1;
     A(i,i+1)=1;A(i+1,i)=1;
     for j=2:n
     A(j,n+2)=1;A(n+2,j)=1;
    end
end
end
A;
```

## 4. CONCLUSIONS

In this paper, MATLAB Program has been presented for computing the Wiener index of some standard graphs. The researcher tested the above program to calculate the Wiener index of above graphs for arbitrary n

## 5. REFERENCES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